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Some of our effort is concerned with the modeling of flames supported by heterogeneous rocket propellants and the modeling of the propellants themselves. We have reported in the past on a number of g-round-breaking contributions that we have made to this subject, and significant new progress has been achieved. We reported last year on a new 3-step kinetics model to replace the earlier 2-step model, and this gives improved agreement with experiental data for burning rates of a variety of heterogeneous propellants. This work has now been publshed:

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1 Objectives

This research is concerned with theoretical studies of combustion and related flow problems that are relevant to the Air Force mission. Recent topics that have been examined include heterogeneous propellant flame modeling, the construction of 1-dimensional flame models from subgrid 3-dimensional descriptions, aluminum agglomeration, the combustion of heterogeneous propellants containing aluminum, the use of a genetic algorithm to optimally define false kinetics parameters in propellant combustion modeling, and instabilities of smolder waves.

2 Personnel

Faculty: John Buckmaster, PI
Post-doctoral student: M.Chen (permanent US resident)

3 Status of effort

Some of our effort is concerned with the modeling of flames supported by heterogeneous rocket propellants and the modeling of the propellants themselves. We have reported in the past on a number of ground-breaking contributions that we have made to this subject, and significant new progress has been achieved. We reported last year on a new 3-step kinetics model to replace the earlier 2-step model, and this gives improved agreement with experiental data for burning rates of a variety of heterogeneous propellants. This work has now been publshed:

1 'New kinetics for a model of heterogeneous propellant combustion', L.Massa, T.L.Jackson, J.Buckmaster *Journal of Propulsion and Power* 21(5), 914-924, 2005. Its abstract is:

In earlier work we describe an unsteady, three-dimensional, phase-coupled combustion code which, with the use of a random packing algorithm to construct model propellants, and the use of a homogenization strategy to account for unresolvably small propellant particles, can be used for the simulation of heterogeneous propellant combustion. This work uses a simple two-step kinetic model for ammonium perchlorate (AP) - hydroxyl terminated polybutadiene (HTPB) combustion which fails to accurately predict variations in the burning rate with AP concentration for a homogenized AP/HTPB blend supporting a one-dimensional flame. Here we describe a three-step model, one which captures the three flames of the Beckstead-Derr-Price (BDP) combustion model, and show that kinetic parameters can be adopted so that one-dimensional AP burning rates and one-dimensional AP/HTBP blend burning rates can be correctly predicted. We discuss the stability of the underlying flame structures, and highlight a difficulty that arises in these instability-prone systems when simple kinetic models are used to describe them. The combustion model, with the new kinetics, is used to reexamine the burning of random packs, and improved agreement with the experimental burning rates of Miller packs is demonstrated. We also reexamine the problem of sandwich-propellant combustion, and investigate the trend in surface shape and burning-rate variations with pressure and binder width. These trends are compared with experimental results of Price. The sandwich

configuration is used to measure the importance of the primary diffusion flame of the BDP model.

We doubt that better agreement with Miller's results could be achieved, and in that sense this paper is a capstone achievement.

Our multi-dimensional computations can not be directly coupled to whole-rocket simulations, because of the difference in scales. They are necessarily subgrid ingredients. A fundamental challenge that we have always faced is how to incorporate our simulations into the whole-rocket simulations, and we have developed a rational strategy for doing this. This work has now been published:

2 'Using heterogeneous propellant burning simulations as subgrid components of rocket simulations', L.Massa, T.L.Jackson, J.Buckmaster *AIAA Journal* 42(9), 1889-1900, 2004. Its abstract is:

We discuss the manner in which 1-dimensional unsteady descriptions can be constructed from multidimensional unsteady simulations of heterogeneous propellant combustion. Spatial averaging of the heat equation within the propellant is used to generate a 1-dimensional equation with a number of source terms defined by the multidimensional thermal field and surface corrugations. Each of these terms is evaluated numerically, and those that may be neglected are identified; models are defined and tested for those that may not. Closure of the 1-dimensional description is achieved by relating the mean surface regression rate and the heat flux from the combustion field at the surface to the pressure and the average surface temperature. These relations are in the form of a look-up table generated from the 'exact' (multidimensional) simulations. The accuracy of the 1-dimensional system is tested by comparing the predictions with those of the exact model. This is done for steady burning rates at various pressures, and for the unsteady burning response to pressure ramps and pressure pulses.

There is a great deal of interest in microscale combustors, as possible replacements for batteries. Wall effects and heat exchange are ingredients that play a much more important role here than in ordinary combustion contexts. One microcombustor configuration of interest is the so-called "swiss roll" combustor, and we have carried out some modeling of this configuration. This has now been published.

3 M.Chen, J.Buckmaster. 'Modelling of combustion and heat transfer in 'Swiss roll' micro-scale combustors'. *Combustion Theory and Modelling*, 8, 701-720, 2004. Its abstract is:

A two-dimensional numerical model is developed to simulate combustion and heat transfer in "Swiss

roll" combustors (SRC). This model couples heat transfer and chemical reaction in the gas and heat diffusion in the conducting walls. The goal of the model is to gain insight into microscale combustion to prevent the occurrence of extinction. In the numerical modeling, the "Swiss roll" geometry is unwrapped into a straight channel, with heat recirculation between the unburned and burned gas properly considered. The simulation is carried out using a fourth-order scheme to discretize the spatial variables, with time integration to steady state based on a first-order Runge-Kutta scheme. We investigate the extinction mechanisms and heat transfer characteristics in the combustor, and perform parametric studies to examine their effects on combustion and extinction. Numerical predictions of extinction limits agree well with experimental data.

Aluminum is often used as an additive in heterogeneous propellants, and one of the most vexing issues for rocket builders is aluminum agglomeration. This refers to the clustering of aluminum particles at the propellant surface prior to detachment. Substantial nozzle scouring and the generation of an identifiable wake are unwanted consequences. We have been able to use the tools that we have developed to examine this problem in a much more sophisticated fashion than hitherto, and the following paper has been published.

4 T.L.Jackson, F.Najjar, J.Buckmaster. 'New aluminum agglomeration models and their use in solid-propellant-rocket simulations'. *Journal of Propulsion and Power* 21(5) 925-936, 2005. Its abstract is:

Random packs of ammonium perchlorate and aluminum particles in fuel binder, of the kind used to mimic the morphology of heterogeneous propellants, define distributions of aluminum particles which can be used as the starting point of agglomeration studies. The goal is to predict the fraction of aluminum that agglomerates, and the size distribution of the agglomerates. Three phenomenological models are described, each with one or two parameters that can be adjusted to fit experimental data, and a number of such fits are attempted. It is shown that the agglomeration models can be calibrated to match a wide variety of propellant outputs, as needed for the numerical simulation of rocket chamber flows with aluminum injection. Results for such flows are presented and provide information about the distribution of the aluminum droplets and of the alumina smoke particles that arises from its presence.

In addition to the agglomeration study of aluminum, we have developed a 3-dimensional combustion code to model propellant combustion in the presence of aluminum particles. A key advance over the non-aluminized work is the necessary use of a sophisticated level-set strategy. The following

paper has been prepared and submitted for publication:

5 X.Wang, T.L.Jackson, J.Buckmaster. 'Numerical simulation of the three-dimensional combustion of aluminized heterogenous propellants'. Submitted. Its abstract is:

We report the first 3-dimensional simulations of aluminized propellant combustion, accounting for heat conduction in the solid, combustion in the gas-phase, and coupling of these via the irregularly moving propellant surface, one that can not be defined by a single-valued height function. The simulations are used to examine the dynamics of aluminum particles in the near-neighborhood of the surface after detachment, and to provide an estimate of the time to ignition of the particles, and their speed and height above the surface at ignition. In addition we examine the temperature history of the particles during their rise to the surface, determine whether they melt or not, and in this way test Cohen's well-known melting criterion. And we discuss a simple model which provides insights into how aluminum particles floating on a binder melt layer would migrate because of surface tension effects, and calculate an average migration distance that is consistent with previous agglomeration studies.

All of our propellant work to date has been concerned with AP/HTPB propellants, with or without aluminum. We are interested in examining other ingredients, including, most importantly, HMX. A major difficulty in the modeling is the specification of the parameters in the global kinetics models that are necessarily used. We have developed an optimization strategy that makes use of a genetic algorithm to deal with this difficulty. The following paper has been prepared and submitted for publication:

6 L.Massa, T.L.Jackson, J.Buckmaster. 'Optimization of global kinetics parameters for heterogeneous propellant combustion using a genetic algorithm'. Submitted. Its abstract is:

We examine the combustion of heterogeneous propellants for which, necessarily, the chemical kinetics is modeled using simple global schemes. Choosing the parameters for such schemes is a significant challenge, one that, in the past, has usually been met using hand-fitting of experimental data (target data) for global burning properties such as steady burning rates, burn-rate temperature sensitivity, and the like. This is an unsatisfactory strategy in many ways. It is not optimal; and if the target set is large and includes such things as stability criteria, or bounds, difficult to implement. Here we discuss the use of a general optimization strategy which can handle large data sets of a general nature. The key numerical tool is a genetic algorithm that uses MPI on a parallel platform. We use this strategy to determine parameters for AP/HTPB propellants and HMX/HTPB propellants. Only 1-dimensional target data is used, corresponding to the burning of pure AP (HMX) or a homogenized blend of fine AP (HMX) and HTPB. The goal is to generate kinetics models that

can be used in the numerical simulation of 3-dimensional heterogeneous propellant combustion. The results of such simulations will be reported in a sequel.

Our (small) interest in smolder combustion survives. In work reported last year on "edge-flames" in smolder we observed instabilities, and so have examined the stability question. A paper has been prepared and submitted for publication:

7 Z.Lu, J.Buckmaster, M.Chen, L.Massa. 'Instabilities of reverse smolder waves'. Submitted. Its abstract is:

We use numerical strategies to examine the stability of reverse smolder waves in the context of a model that can permit both fuel-rich and fuel-lean waves. The steady-state response for such waves, maximum temperature versus blowing rate, is characterized, for increasing blowing rate, by a fuel-rich branch of rising temperature followed by a fuel-lean branch of falling temperature, followed by quenching. The propagation speed at the quenching point is nonzero. For the parameters that we consider, the entire fuel-rich branch is unstable to 2-dimensional disturbances, but the dynamic consequences are modest. An interval of the fuel-lean branch whose left boundary is at the point of stoichiometry is stable, but the remainder of the branch, all the way to the quenching point, is unstable. These instabilities are destructive, and the contiguous smolder wave becomes fragmented. Tribrachial fragments can emerge, analagous to the tribrachial or triple flames familiar from gaseous edge-flame studies. Their emergence is characterized by a sharp rise in the maximum temperature, a rise that could lead to a transition to flaming (gas-phase) combustion.

4 Public service

- The PI is on the editorial board of the journal *Combustion Theory and Modelling.*

5 Honors

- Senior U.S. Scientist Award (Humboldt Prize), 1985, 1986
  Buckmaster, J.

Alexander von Humboldt Foundation, Germany

- JSPS Fellow, 1986
  Buckmaster, J.
  Japan Society for the Promotion of Science, Japan

- Fellow, American Physical Society, 1986
  Buckmaster, J.
  American Physical Society, USA

- Guggenheim Fellowship, 1990
  Buckmaster, J.
  Guggenheim Foundation, USA

- Fellow of the Institute of Physics (UK), and Chartered Physicist, 1999
  Buckmaster, J.

- AIAA Propellants and Combustion Award for 2002, "for outstanding theoretical contributions to the physical understanding of fluid mechanics in combustion processes ranging from detonation physics to propellants", 2002
  Buckmaster,J.
  American Institute of Aeronautics and Astronautics, USA

- Zeldovich Gold Medal of the Combustion Institute for 2004, "for outstanding contribution to the theory of combustion".

6 Other activity

The PI is a participant in a DOE ASCI center, concerned with solid propellant rocket motors, centered in the Computer Science and Engineering program of the University of Illinois. He provides guidance in the context of propellant flame physics and chemistry. His collaborative work with T.L.Jackson, a senior research scientist in the center, comes about because of this.